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Applied Math Research Program Update

Homer Walker

ASCR Advisory Committee Meeting
Gaithersburg, MD
November 6, 2007

Applied Math Program

- **Research on the mathematical methods and numerical algorithms that enable the effective description, understanding, and prediction of complex physical, biological, and human-engineered systems.**

- **Current research support includes**
  - ***PDEs, ODEs, dynamical systems***
  - ***linear and nonlinear solvers***
  - ***optimization***
  - ***meshing***
  - ***computational fluid dynamics***
  - ***multiscale mathematics***

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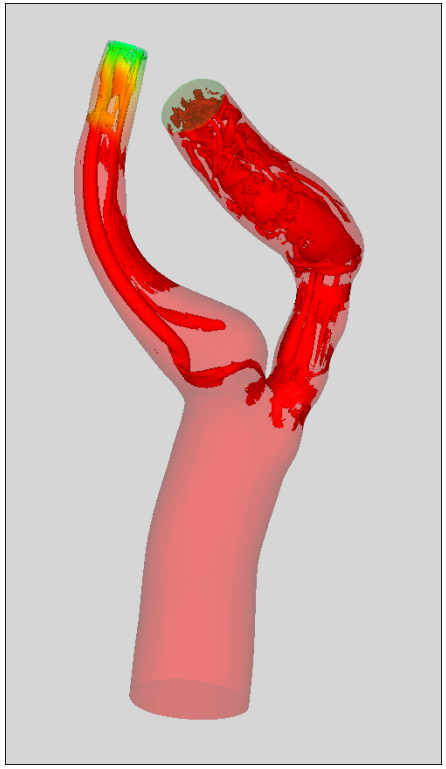
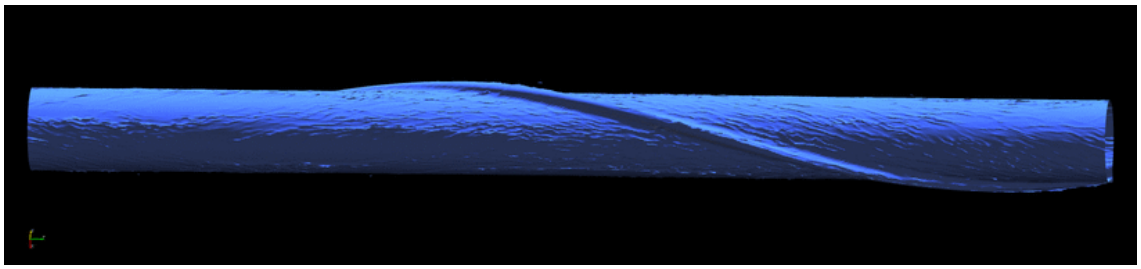
Highlighted FY07 Accomplishment

Paul Fischer, ANL

Nek5000 Applications Pave the Way to Petascale

- **Spectral-element multigrid code with parallel coarse-grid solver**
- **Scales to petascale platforms**
- **Previously shared the 1999 Gordon Bell Prize (Special Category)**
- **2007 accomplishments include**
  - ***Magnetorotational instabilities (MRI) simulations***
  - ***Reactor thermal-hydraulics simulations (below)***
  - ***Turbulent vascular flow simulations (right)***





Above: coherent structures arising near a carotid artery with severe stenosis, Re = 1400. Simulations performed on ANL's IBM BGL using 1024 processors. Featured in NY Times article

Left: turbulent flow past a wire-wrapped fuel pin in a liquid metal-cooled reactor (iso-surface of axial velocity component). Note the turbulence-induced low-speed streaks reaching from the boundary layer into the bulk flow domain.

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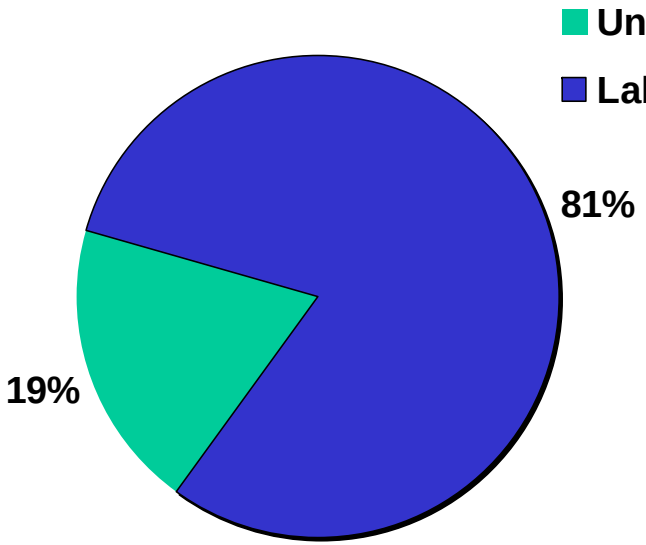
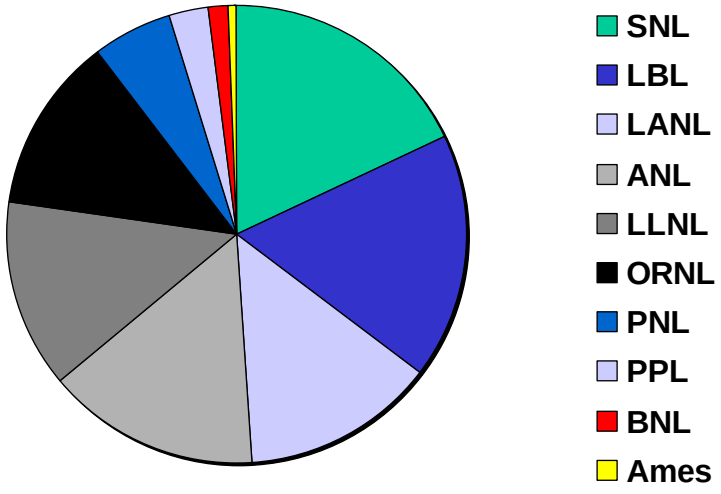
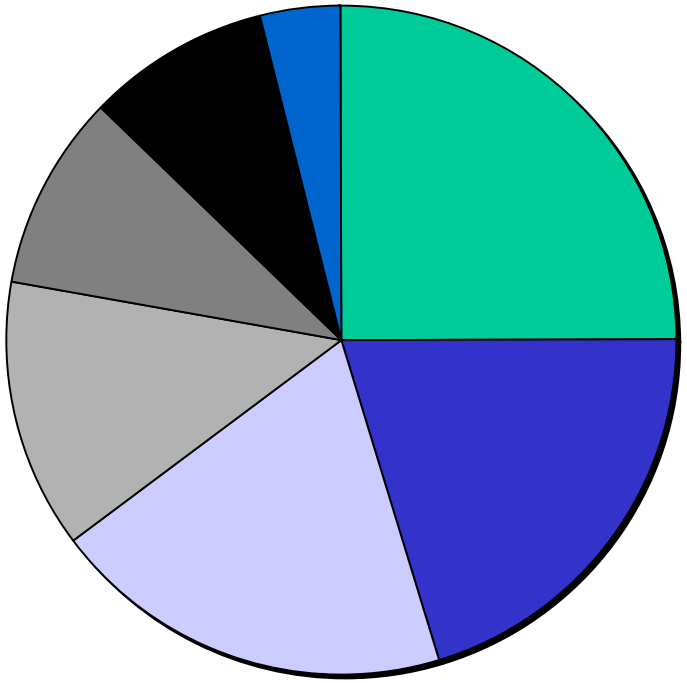
Current FY08 Plan





- **Based on $22.4M**
- **Does not include awards delayed by the continuing resolution**
- **Does not include $5M for CSGF**

Allocations by Area



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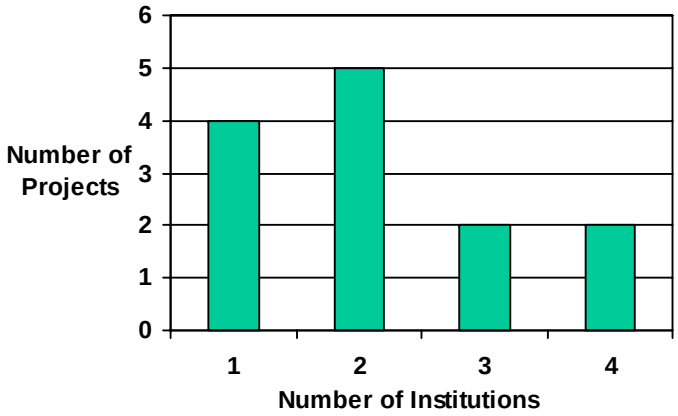
Multiscale Mathematics Research & Education

- **2005 announcement**
  - *Advancement of multiscale mathematics research*
  - *Innovative approaches to multiscale mathematics education*
  - *Inter-institutional collaboration encouraged*
  - *Up to $5.8M anticipated in FY05*

- **13 projects, 28 institutions funded**
  - *$5.6M planned for FY08*
  - *Almost all will terminate in 8/08*



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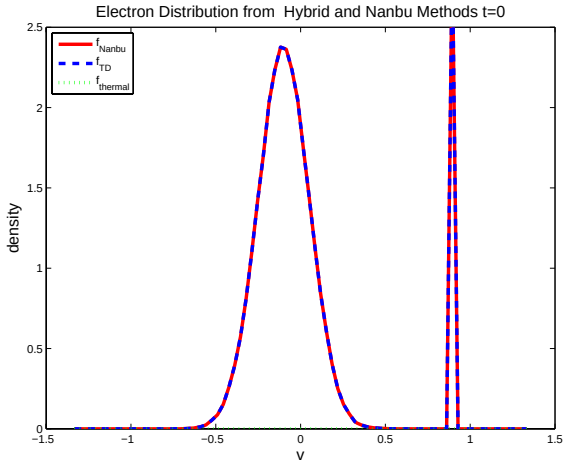
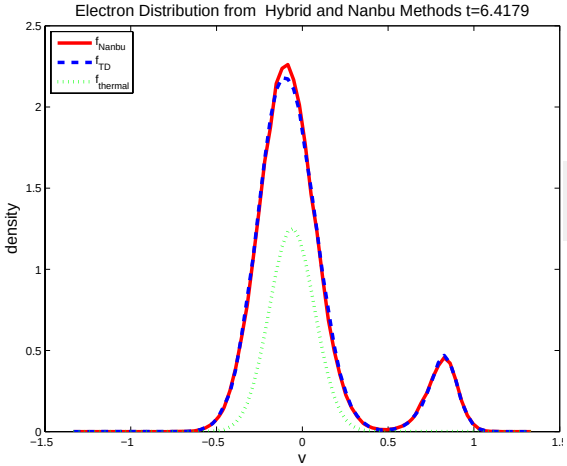
Highlighted FY07 MM Accomplishment

UCLA (R. Caflisch, R. Wang), LLNL (A. Dimits, B. Cohen)

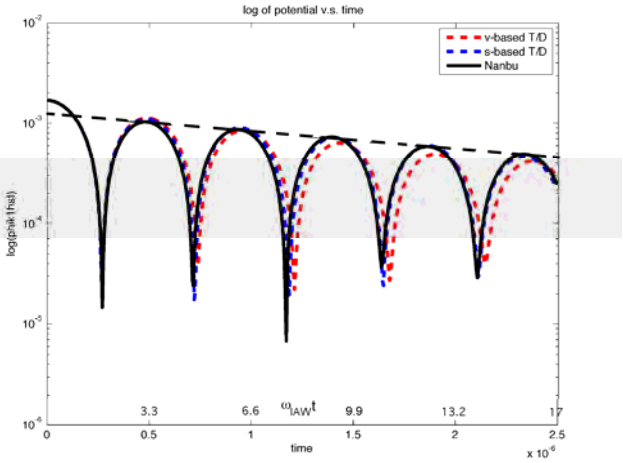
Multiscale Mathematics for Plasma Kinetics Spanning Multiple Collisionality Regimes

- **Motivation:** Wide range of collisional time scales are a major bottleneck for plasma simulations
- **Goals:** Accelerated methods that combine multiple time and length scales for Coulomb collisions
- **Results:** A hybrid particle/continuum method and applications to test problems.





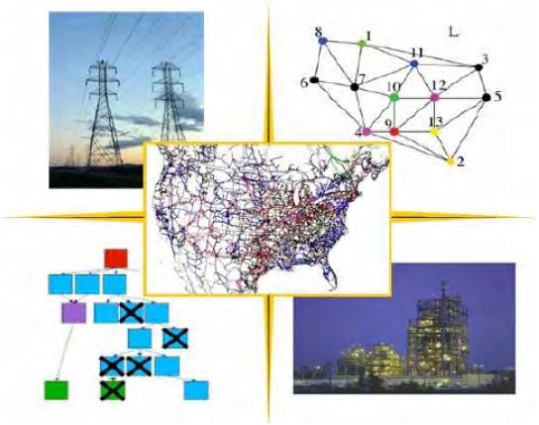
Velocity distributions initially (left) and at t = 6.4179 (right). The blue curve is from the hybrid method; the red is from the standard "exact" method.



Oscillation and decay of ion acoustic waves.

Upcoming

- **Announcement**
  - **continuation of multiscale mathematics**
  - **optimization of complex systems**
    - ***Many components (possibly dissimilar), complex connectivity (usually nonlinear), hard-to-predict behavior (often highly sensitive)***
    - ***Examples: power grid control and optimization, the nuclear fuel lifecycle, fossil fuel power generation, risk assessment for cybersecurity***
    - ***New mathematical insights needed in modeling, large-scale mixed-variable optimization, sensitivity and risk analysis, statistical methods for validation, integration of models with data for adaptive control and decision making***



From "Mathematical Research Challenges in Optimization of Comples Systems," report on a DOE Workshop, December 7-8, 2006, organizers Bruce A. Hendrickson and Margaret H. Wright.

Upcoming (cont.)

- **Applied Math PI meeting**
- **Workshop on mathematics for understanding petascale data sets**
  - ***R. L. Orbach AAAS talk, Feb. 2006, "New Opportunities for Data and Information management: Finding the Dots, Connecting the Dots, Understanding the Dots"***
  - ***Need innovative mathematical approaches and techniques for finding the scientific knowledge in massive, complex data sets***
  - ***Workshop goals: understand the needs of various scientific domains, translate these into mathematical approaches and techniques, assess the current state-of-the-art, target gaps and shortfalls that must be addressed.***
  - ***Resonates with activities at NSF and DARPA.***
- **Strategic plan**
  - ***Informed by the report of a panel chaired by David Brown to assess DOE challenges and opportunities in applied and computational mathematics***